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research note

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Date: March 13, 1998

Adaptation of Booth's Monte Carlo Transport Estimation, in $[x, \mu]$ Geometry, to the Reduced Source Method

Abstract

Booth has described how the parameters for the analytic form of the transport solution, to the one speed finite slab problem in $[x, \mu]$ geometry, can be estimated by Monte Carlo. The research documented herein concerns the extension to the reduced-source method of Booth's approach. The reduced-source method is an iterative calculational approach that is believed to result in a roughly exponential rate of convergence to the exact solution, constrained only by the precision of numerical algorithms and finite computer word-length.

Preface

Manipulation of the equations within this note draw from, and presuppose a familiarity with, Tom Booth's (X-CI) paper,[1] which has been submitted to the American Nuclear Society for publication. In addition, the resulting adapted FORTRAN test-bed code is a generalization of Booth's original test-bed code, named "xmuh" (*i.e.*, "$[x, \mu]$-geometry code for Henry"). The reduced-source method has been described recently by Gregg McKinney (X-CI).[2]

1. Introduction

In order to focus attention on that which is new in the present document, the starting point for this research is presented in this section with a minimum of discussion. That is, Equations 1–10, below, are presented for convenience, but are neither derived nor discussed herein, except for some basic definitions of terms.

Booth starts his own derivation with Case's method, following the notation in Bell and Glasstone.[3] The analytic form of the transport solution, to the one speed finite slab problem in $[x, \mu]$ geometry (with isotropic scattering), is given by

$$\Phi(x, \mu) = a_+ \psi_0^+(\mu) e^{-x/\nu_0} + a_- \psi_0^-(\mu) e^{x/\nu_0} + \int_{-1}^{1} A(\nu) \psi_\nu(\mu) e^{-x/\nu} d\nu \qquad (1)$$

where

x is the spatial position (measured along the slab normal);

μ is the direction cosine with respect to the x-axis;

$\Phi(x,\mu)$ is the angular flux;

$\pm\nu_0$ are the discrete eigenvalues of the associated eigenfunctions

$$\psi_0^{\pm}(\mu) = \frac{c}{2}\frac{\nu_0}{\nu_0 \mp \mu} \tag{2}$$

with

ν_0 being the positive root of

$$1 = c\nu_0 tanh^{-1}\frac{1}{\nu_0} \equiv \frac{c\nu_0}{2} ln\frac{\nu_0+1}{\nu_0-1} \tag{3}$$

ν is an eigenvalue corresponding to the eigenfunction

$$\psi_\nu(\mu) = \frac{c}{2}P\frac{\nu}{\nu-\mu} + \lambda(\nu)\delta(\mu-\nu) \tag{4}$$

$$\lambda(\nu) = 1 - \frac{c\nu}{2} ln\Big(\frac{1+\nu}{1-\nu}\Big) \tag{5}$$

where

c is (for non-multiplying media) the collision survival probability;

P indicates that the Cauchy principal value is to be used in any integration of a singular term;

and

$\delta(x)$ is the Dirac delta function.

From the orthogonality conditions on $\psi_0^{\pm}(\mu)$ and $\psi_\nu(\mu)$

$$a_{\pm} = \frac{1}{N_0^{\pm}}\int_{-1}^{1}\Phi(0,\mu)\mu\psi_0^{\pm}(\mu)d\mu \tag{6}$$

$$A(\nu) = \frac{1}{N_\nu}\int_{-1}^{1}\Phi(0,\mu)\mu\psi_\nu(\mu)d\mu \tag{7}$$

where

$$N_0^{\pm} = \int_{-1}^{1} \mu \psi_0^{\pm}(\mu) \psi_0^{\pm}(\mu) d\mu = \pm \frac{c}{2} \nu_0^3 \Big[\frac{c}{\nu_0^2 - 1} - \frac{1}{\nu_0^2} \Big] \tag{8}$$

$$\int_{-1}^{1} \mu \psi_{\nu'}(\mu) \psi_{\nu}(\mu) d\mu = N_{\nu} \delta(\nu - \nu') \tag{9}$$

$$N_{\nu} = \nu \Big[\lambda^2(\nu) + \frac{\pi^2 c^2}{4} \nu^2 \Big] \tag{10}$$

Based on the forgoing, Booth derives and prescribes[1] Monte Carlo estimation for quantities that are used to obtain the coefficients $A(\nu)$ in Equation 7. These, together with all the other computed quantities specified in Equations 2–10, are used to obtain the flux specified in Equation 1.

2. The Reduced Source at the Boundary

If the slab thickness is T, then the left and right boundaries may be specified as $x = 0$ and $x = T$, or, equivalently, as $x = -T$ and $x = 0$, respectively. We will have use for both specifications (just as Booth explained in Reference [1], Section IV): the former specification for left-boundary computations; the latter for right boundary computations.

Given the computed angular flux, $\Phi(x, \mu)$, at the slab boundaries (initially choosing $x = 0$ to be the left boundary and $x = T$ the right), the corresponding boundary source-density is given by

$$S(\mu) = \mid \mu \mid [\Phi(0, \mu) H(\mu) + \Phi(T, \mu) H(-\mu)] \tag{11}$$

where $H(z) = \int_{-\infty}^{z} \delta(y) dy$ is the Heaviside function, and $\Phi(x, \mu)$ is given by Equation 1.

If the computed value of $\Phi(x, \mu)$, say $\Phi^1(x, \mu)$, is equal to the exact solution for the given problem, say $\Phi^E(x, \mu)$, then $S(\mu)$ will be exactly equal to the given source at the boundary, say $S^E(\mu)$. As Booth points out (Reference [1], Section VIII), "If there were a *perfect* match at the boundary, then the estimated solution would be identical to the true solution by uniqueness.[4] That is, the estimated solution would then *exactly* satisfy both the transport equation and the boundary conditions."

Any non-vanishing *algebraic* difference between the given source, $S^E(\mu)$, and the computed source, from Equation 11, comprises the reduced source at the boundary, or boundary residual,

$$S^1(\mu) = S^E(\mu) - S(\mu) \tag{12}$$

$S^1(\mu)$, in turn, specifies the source for the problem, whose solution, say $\Phi^2(x,\mu)$, is the difference between the exact solution to the original problem and the solution given by $\Phi^1(x,\mu)$, *viz.*

$$\Phi^E(x,\mu) = \Phi^1(x,\mu) + \Phi^2(x,\mu) \tag{13}$$

It should be noted that $S^1(\mu)$ can and, in practice, does have both positive and negative components. This is treated by assigning positive and negative weights, respectively, in the subsequent Monte Carlo estimation.

If $\Phi^2(x,\mu)$ is not an *exact* solution (to the problem for which $S^1(\mu)$ is the given source), as would be evidenced by a *sufficiently* large boundary residual, say $S^2(\mu)$, the process can be continued for another iteration. The choice of a termination criterion, based on a specified magnitude of boundary residual, is arbitrary.

In this manner, Equations 11–13 prescribe an iterative method for converging to the exact solution of the original problem — the reduced-source method.

3. Components of Transport Coefficients Due to Boundary Residual

The components of the transport coefficients, due to the *direct* contribution from the boundary residual of Equation 12, can be computed by numerical integration (Reference [1], Appendix). The remaining components (*i.e., not* due to the direct contribution from the boundary residual) are estimated as Booth prescribed and coded in xmuh.

3.1 Components due to left-boundary residual

Subscripting with L to indicate left-boundary quantities, the left-boundary flux due to the left-boundary residual source density is, from Equations 11 and 12

$$\phi_L(\mu)H(\mu) = \frac{S_L^1(\mu)}{\mid \mu \mid} = \frac{S_L^E(\mu)}{\mid \mu \mid} - \Phi(0,\mu)H(\mu) \tag{14}$$

where $S_L^E(\mu)$ is the given source (on the left boundary) and $\Phi(0,\mu)$ is the computed flux (on the left boundary).

3.1.1 $A(\nu)$ due to left-boundary residual:

Substituting Equation 14 into Equation 7 we get

$$A_L(\nu) = \frac{1}{N_\nu}\int_{-1}^{1} \phi_L(\mu)H(\mu)\mu\psi_\nu(\mu)d\mu \tag{15}$$

Using Equations 4 and 15 we get

$$\begin{aligned} A_L(\nu) &= \frac{1}{N_\nu}\int_{-1}^{1}\phi_L(\mu)H(\mu)\mu\Big[\frac{c}{2}P\frac{\nu}{\nu-\mu}+\lambda(\nu)\delta(\mu-\nu)\Big]d\mu \\ &= \frac{1}{N_\nu}\int_{0}^{1}\phi_L(\mu)\mu\frac{c}{2}P\frac{\nu}{\nu-\mu}d\mu+\frac{1}{N_\nu}\phi_L(\nu)H(\nu)\nu\lambda(\nu) \\ &= I_L(\nu)+B_L(\nu) \end{aligned} \tag{16}$$

where

$$I_L(\nu)=\frac{1}{N_\nu}\int_{0}^{1}\phi_L(\mu)\mu\frac{c}{2}P\frac{\nu}{\nu-\mu}d\mu \tag{17}$$

and

$$B_L(\nu)=\frac{1}{N_\nu}\phi_L(\nu)H(\nu)\nu\lambda(\nu) \tag{18}$$

Using Equations 10 and 18 we get

$$\begin{aligned} B_L(\nu) &= \frac{\phi_L(\nu)H(\nu)\nu\lambda(\nu)}{\nu\Big[\lambda^2(\nu)+\frac{\pi^2c^2}{4}\nu^2\Big]} \\ &= \frac{\phi_L(\nu)H(\nu)}{\Big[\lambda(\nu)+\frac{\pi^2c^2}{4\lambda(\nu)}\nu^2\Big]} \end{aligned} \tag{19}$$

From Equation 5, we see that $\lambda(\nu)$ is unbounded for $\nu=\pm1$; but, $B_L(\pm1)$ vanishes, as can be seen from Equation 19.

The $I_L(\nu)$ of Equation 17 can be calculated, with appropriate care in the vicinity of $\nu=\mu$, using the approach in Reference [1], Section VII. And, as Booth explains in Reference [1], Section IV, we need $A_L(\nu)$ only for $\nu>0$, and, conversely, we need $A(\nu)$ on the right boundary, $A_R(\nu)$, only for $\nu<0$ (see Section 3.2, below).

Divide the interval [-1,1] into $2K$ equal intervals, and, for $0\le\nu\le1$, let ν_i and μ_i be the midpoints of the intervals

$$\mu_i=\nu_i=\frac{(i-\frac{1}{2})-K}{K} \qquad i=K+1,K+2,\cdots,2K \tag{20}$$

Let

$$l_i = \frac{i-K}{K} \qquad i = K+1, K+2, \cdots, 2K \tag{21}$$

be the endpoints of the i^{th} interval, *viz.*

$$l_{i-1} \leq \nu < l_i \qquad i = K+1, K+2, \cdots, 2K \tag{22}$$

To evaluate $I_L(\nu)$ for the eigenvalues ν_j, assume a linear form for

$$\alpha(\mu) = \frac{1}{2N_\nu}\phi_L(\mu)c\mu\nu \tag{23}$$

in each interval. That is,

$$\alpha_i(\mu) = a_i(\nu_j - \mu) + c_i \qquad i = K+1, K+2, \cdots, 2K \tag{24}$$

Note that a_i in Equation 24 is the slope of our linearized $\alpha_i(\mu)$ in each interval. For $i = K+1$ and $i = 2K$ we use a one-sided estimate of the a_i, because no information about $\phi_L(\mu)H(\mu)$ exists for $i = K$ or $i = 2K+1$. Elsewhere, a two-sided estimate of the slope is used.

Hence

$$a_{K+1} = \frac{\alpha(\mu_{K+2}) - \alpha(\mu_{K+1})}{\mu_{K+1} - \mu_{K+2}} = K[\alpha(\mu_{K+1}) - \alpha(\mu_{K+2})] \tag{25}$$

$$c_{K+1} = \alpha(\mu_{K+1}) - a_{K+1}(\nu_j - \mu_{K+1}) \tag{26}$$

$$a_i = \frac{\alpha(\mu_{i+1}) - \alpha(\mu_{i-1})}{\mu_{i-1} - \mu_{i+1}} = \frac{K}{2}[\alpha(\mu_{i-1}) - \alpha(\mu_{i+1})] \qquad i = K+2, K+3, \cdots, 2K-1 \tag{27}$$

$$c_i = \alpha(\mu_i) - a_i(\nu_j - \mu_i) \qquad i = K+2, K+3, \cdots, 2K-1 \tag{28}$$

$$a_{2K} = \frac{\alpha(\mu_{2K}) - \alpha(\mu_{2K-1})}{\mu_{2K-1} - \mu_{2K}} = K[\alpha(\mu_{2K-1}) - \alpha(\mu_{2K})] \tag{29}$$

$$c_{2K} = \alpha(\mu_{2K}) - a_{2K}(\nu_j - \mu_{2K}) \tag{30}$$

Thus, in the i^{th} interval, we get from Equation 17 and the Definitions 20–30

$$\begin{aligned} I_L^i(\nu_j) &= \int_{l_{i-1}}^{l_i} \frac{a_i(\nu_j - \mu) + c_i}{\nu_j - \mu} d\mu \\ &= a_i(l_i - l_{i-1}) + c_i \int_{l_{i-1}}^{l_i} \frac{1}{\nu_j - \mu} d\mu \\ &= \frac{a_i}{K} + c_i ln\left|\frac{\nu_j - l_{i-1}}{\nu_j - l_i}\right| \end{aligned} \tag{31}$$

And note that for the case of $i = j$ we have

$$ln\left|\frac{\nu_j - l_{i-1}}{\nu_j - l_i}\right| = ln\left|\frac{\nu_j - l_{j-1}}{\nu_j - l_j}\right| = ln\left|\frac{\frac{1}{2K}}{\frac{-1}{2K}}\right| = ln(1) = 0 \tag{32}$$

so that

$$I_L^j(\nu_j) = \frac{a_j}{K} \tag{33}$$

Hence, the value of $I_L(\nu)$ in Equation 17 can be approximated for $\nu = \nu_j$ such that

$$I_L(\nu) \simeq \sum_{i=K+1}^{2K} I_L^i(\nu_j) \tag{34}$$

3.1.2 a_+ due to left-boundary residual:

Substituting Equation 14 into Equation 6 (for a_+) we get

$$a_+ = \frac{1}{N_0^+} \int_{-1}^{1} \phi_L(\mu) H(\mu) \mu \psi_0^+(\mu) d\mu \tag{35}$$

Using Equation 2, Equation 35 becomes

$$\begin{aligned} a_+ &= \frac{1}{N_0^+} \int_{-1}^{1} \phi_L(\mu) H(\mu) \mu \frac{c}{2} \frac{\nu_0}{\nu_0 - \mu} d\mu \\ &= \frac{c\nu_0}{2N_0^+} \int_0^1 \frac{\phi_L(\mu)\mu}{\nu_0 - \mu} d\mu \end{aligned} \tag{36}$$

where we note that $\nu_0 > 1$ (Reference [3], page 72).

Following the approach in Section 3.1.1 above, assume a linear form for

$$\alpha(\mu) = \frac{c\nu_0\phi_L(\mu)\mu}{2N_0^+} \tag{37}$$

in each interval i such that

$$\alpha_i(\mu) = a_i(\nu_0 - \mu) + c_i \qquad i = K+1, K+2, \cdots, 2K \tag{38}$$

where

$$a_{K+1} = \frac{\alpha(\mu_{K+2}) - \alpha(\mu_{K+1})}{\mu_{K+1} - \mu_{K+2}} = K[\alpha(\mu_{K+1}) - \alpha(\mu_{K+2})] \tag{39}$$

$$c_{K+1} = \alpha(\mu_{K+1}) - a_{K+1}(\nu_0 - \mu_{K+1}) \tag{40}$$

$$a_i = \frac{\alpha(\mu_{i+1}) - \alpha(\mu_{i-1})}{\mu_{i-1} - \mu_{i+1}} = \frac{K}{2}[\alpha(\mu_{i-1}) - \alpha(\mu_{i+1})] \qquad i = K+2, K+3, \cdots, 2K-1 \tag{41}$$

$$c_i = \alpha(\mu_i) - a_i(\nu_0 - \mu_i) \qquad i = K+2, K+3, \cdots, 2K-1 \tag{42}$$

$$a_{2K} = \frac{\alpha(\mu_{2K}) - \alpha(\mu_{2K-1})}{\mu_{2K-1} - \mu_{2K}} = K[\alpha(\mu_{2K-1}) - \alpha(\mu_{2K})] \tag{43}$$

$$c_{2K} = \alpha(\mu_{2K}) - a_{2K}(\nu_0 - \mu_{2K}) \tag{44}$$

Then

$$\begin{aligned} a_+^i &= \int_{l_{i-1}}^{l_i} \frac{a_i(\nu_0 - \mu) + c_i}{\nu_0 - \mu} d\mu \\ &= \frac{a_i}{K} + c_i ln\left(\frac{\nu_0 - l_{i-1}}{\nu_0 - l_i}\right) \end{aligned} \tag{45}$$

and a_+ is approximated by

$$a_+ \simeq \sum_{i=K+1}^{2K} a_+^i \tag{46}$$

3.2 Components due to right-boundary residual

We now choose $x = -T$ to be the left boundary and $x = 0$ the right. Then the boundary source-density as given by Equation 11 is now written as

$$S(\mu) = \mid \mu \mid [\Phi(-T, \mu)H(\mu) + \Phi(0, \mu)H(-\mu)] \tag{47}$$

Subscripting with R to indicate right-boundary quantities, the right-boundary flux due to the right-boundary residual source density is, from Equations 47 and 12

$$\phi_R(\mu)H(-\mu) = \frac{S_R^1(\mu)}{\mid \mu \mid} = \frac{S_R^E(\mu)}{\mid \mu \mid} - \Phi(0, \mu)H(-\mu) \tag{48}$$

where $S_R^E(\mu)$ is the given source (if any, on the right boundary), and $\Phi(0, \mu)$ is the computed flux (on the right boundary).

3.2.1 $A(\nu)$ due to right-boundary residual:

Substituting Equation 48 into Equation 7 we get

$$A_R(\nu) = \frac{1}{N_\nu} \int_{-1}^{1} \phi_R(\mu)H(-\mu)\mu\psi_\nu(\mu)d\mu \tag{49}$$

Using Equations 4 and 49 we get

$$\begin{aligned} A_R(\nu) &= \frac{1}{N_\nu} \int_{-1}^{1} \phi_R(\mu)H(-\mu)\mu\Big[\frac{c}{2}P\frac{\nu}{\nu - \mu} + \lambda(\nu)\delta(\mu - \nu)\Big]d\mu \\ &= \frac{1}{N_\nu} \int_{-1}^{0} \phi_R(\mu)\mu\frac{c}{2}P\frac{\nu}{\nu - \mu}d\mu + \frac{1}{N_\nu}\phi_R(\nu)H(-\nu)\nu\lambda(\nu) \\ &= I_R(\nu) + B_R(\nu) \end{aligned} \tag{50}$$

where

$$I_R(\nu) = \frac{1}{N_\nu} \int_{-1}^{0} \phi_R(\mu)\mu\frac{c}{2}P\frac{\nu}{\nu - \mu}d\mu \tag{51}$$

and

$$B_R(\nu) = \frac{1}{N_\nu}\phi_R(\nu)H(-\nu)\nu\lambda(\nu) \tag{52}$$

Using Equations 10 and 52 we get

$$\begin{aligned} B_R(\nu) &= \frac{\phi_R(\nu)H(-\nu)\nu\lambda(\nu)}{\nu\left[\lambda^2(\nu)+\frac{\pi^2c^2}{4}\nu^2\right]} \\ &= \frac{\phi_R(\nu)H(-\nu)}{\left[\lambda(\nu)+\frac{\pi^2c^2}{4\lambda(\nu)}\nu^2\right]} \end{aligned} \tag{53}$$

From Equation 5, we see that $\lambda(\nu)$ is unbounded for $\nu = \pm 1$; but, $B_R(\pm 1)$ vanishes, as can be seen from Equation 53.

The $I_R(\nu)$ of Equation 51 can be calculated, with appropriate care in the vicinity of $\nu = \mu$, using the approach in Section 3.1.1, above. And again, as Booth explains in Reference [1], Section IV, we need $A_R(\nu)$ only for $\nu < 0$.

Divide the interval [-1,1] into $2K$ equal intervals (same as in Section 3.1.1, above), and, for $-1 \leq \nu \leq 0$, let ν_i and μ_i be the midpoints of the intervals

$$\mu_i = \nu_i = \frac{(i-\frac{1}{2})-K}{K} \qquad i = 1, 2, \cdots, K \tag{54}$$

Let

$$l_i = \frac{i-K}{K} \qquad i = 1, 2, \cdots, K \tag{55}$$

be the endpoints of the i^{th} interval, *viz.*

$$l_{i-1} \leq \nu < l_i \qquad i = 1, 2, \cdots, K \tag{56}$$

To evaluate $I_R(\nu)$ for the eigenvalues ν_j, assume a linear form for

$$\alpha(\mu) = \frac{1}{2N_\nu}\phi_R(\mu)c\mu\nu \tag{57}$$

in each interval. That is,

$$\alpha_i(\mu) = a_i(\nu_j - \mu) + c_i \qquad i = 1, 2, \cdots, K \tag{58}$$

Note that a_i in Equation 58 is the slope of our linearized $\alpha_i(\mu)$ in each interval. For $i = 1$ and $i = K$ we use a one-sided estimate of the a_i, because no information about $\phi_R(\mu)H(-\mu)$ exists for $i = 0$ or $i = K + 1$. Elsewhere, a two-sided estimate of the slope is used.

Hence

$$a_1 = \frac{\alpha(\mu_2) - \alpha(\mu_1)}{\mu_1 - \mu_2} = K[\alpha(\mu_1) - \alpha(\mu_2)] \tag{59}$$

$$c_1 = \alpha(\mu_1) - a_1(\nu_j - \mu_1) \tag{60}$$

$$a_i = \frac{\alpha(\mu_{i+1}) - \alpha(\mu_{i-1})}{\mu_{i-1} - \mu_{i+1}} = \frac{K}{2}[\alpha(\mu_{i-1}) - \alpha(\mu_{i+1})] \qquad i = 2, 3, \cdots, K-1 \tag{61}$$

$$c_i = \alpha(\mu_i) - a_i(\nu_j - \mu_i) \qquad i = 2, 3, \cdots, K-1 \tag{62}$$

$$a_K = \frac{\alpha(\mu_K) - \alpha(\mu_{K-1})}{\mu_{K-1} - \mu_K} = K[\alpha(\mu_{K-1}) - \alpha(\mu_K)] \tag{63}$$

$$c_K = \alpha(\mu_K) - a_K(\nu_j - \mu_K) \tag{64}$$

Thus, in the i^{th} interval, we get from Equation 51 and the Definitions 54–64

$$\begin{aligned} I_R^i(\nu_j) &= \int_{l_{i-1}}^{l_i} \frac{a_i(\nu_j - \mu) + c_i}{\nu_j - \mu} d\mu \\ &= a_i(l_i - l_{i-1}) + c_i \int_{l_{i-1}}^{l_i} \frac{1}{\nu_j - \mu} d\mu \\ &= \frac{a_i}{K} + c_i ln\left|\frac{\nu_j - l_{i-1}}{\nu_j - l_i}\right| \end{aligned} \tag{65}$$

And note that for the case of $i = j$ we have

$$ln\left|\frac{\nu_j - l_{i-1}}{\nu_j - l_i}\right| = ln\left|\frac{\nu_j - l_{j-1}}{\nu_j - l_j}\right| = ln\left|\frac{\frac{1}{2K}}{\frac{-1}{2K}}\right| = ln(1) = 0 \tag{66}$$

so that

$$I_R^j(\nu_j) = \frac{a_j}{K} \tag{67}$$

Hence, the value of $I_R(\nu)$ in Equation 51 can be approximated for $\nu = \nu_j$ such that

$$I_R(\nu) \simeq \sum_{i=1}^{K} I_R^i(\nu_j) \tag{68}$$

3.2.2 a_- due to right-boundary residual:

Substituting Equation 48 into Equation 6 (for a_-) we get

$$a_- = \frac{1}{N_0^-} \int_{-1}^{1} \phi_R(\mu) H(-\mu) \mu \psi_0^-(\mu) d\mu \tag{69}$$

Using Equation 2, Equation 69 becomes

$$\begin{aligned} a_- &= \frac{1}{N_0^-} \int_{-1}^{1} \phi_R(\mu) H(-\mu) \mu \frac{c}{2} \frac{\nu_0}{\nu_0 + \mu} d\mu \\ &= \frac{c\nu_0}{2N_0^-} \int_{-1}^{0} \frac{\phi_R(\mu)\mu}{\nu_0 + \mu} d\mu \end{aligned} \tag{70}$$

where, again, we note that $\nu_0 > 1$ (Reference [3], page 72).

Following the approach in Section 3.1.2 above, assume a linear form for

$$\alpha(\mu) = \frac{c\nu_0 \phi_R(\mu)\mu}{2N_0^-} \tag{71}$$

in each interval i such that

$$\alpha_i(\mu) = a_i(\nu_0 + \mu) + c_i \qquad i = 1, 2, \cdots, K \tag{72}$$

where

$$a_1 = \frac{\alpha(\mu_2) - \alpha(\mu_1)}{\mu_2 - \mu_1} = K[\alpha(\mu_2) - \alpha(\mu_1)] \tag{73}$$

$$c_1 = \alpha(\mu_1) - a_1(\nu_0 + \mu_1) \tag{74}$$

$$a_i = \frac{\alpha(\mu_{i+1}) - \alpha(\mu_{i-1})}{\mu_{i+1} - \mu_{i-1}} = \frac{K}{2}[\alpha(\mu_{i+1}) - \alpha(\mu_{i-1})] \qquad i = 2, 3, \cdots, K-1 \tag{75}$$

$$c_i = \alpha(\mu_i) - a_i(\nu_0 + \mu_i) \qquad i = 2, 3, \cdots, K-1 \tag{76}$$

$$a_K = \frac{\alpha(\mu_K) - \alpha(\mu_{K-1})}{\mu_K - \mu_{K-1}} = K[\alpha(\mu_K) - \alpha(\mu_{K-1})] \tag{77}$$

$$c_K = \alpha(\mu_K) - a_K(\nu_0 + \mu_K) \tag{78}$$

Then

$$\begin{aligned} a_-^i &= \int_{l_{i-1}}^{l_i} \frac{a_i(\nu_0 + \mu) + c_i}{\nu_0 + \mu} d\mu \\ &= \frac{a_i}{K} + c_i ln\left(\frac{\nu_0 + l_i}{\nu_0 + l_{i-1}}\right) \end{aligned} \tag{79}$$

and a_- is approximated by

$$a_- \simeq \sum_{i=1}^{K} a_-^i \tag{80}$$

4. Implementation of Reduced Source Algorithms into Test-bed Code

The implementation of the algorithms implied by the foregoing sections is straightforward to describe. What is required, essentially, is:

1. an iteration loop surrounding Booth's Monte Carlo estimation (originally designed for one pass of a specified number of histories);
2. the coding that computes the reduced source at the end of each iteration (see Section 2, above);
3. coding to sample the reduced source (which, in general, will have both positive and negative components on both sides of the slab);
4. coding that computes, by numerical integration, the *direct* reduced-source contributions to the transport coefficients (see Section 3, above).

The devil is in the details, however.

Just as traditional Monte Carlo coding is prone to having bugs that are sometimes difficult to uncover, the intricacies of reduced-source iteration seem to exacerbate such difficulties. And the introduction of negative sources, which stem from overprediction of the boundary sources in a precursor iteration, add more mud to the already muddy waters. One can imagine all the opportunities provided by the foregoing eighty or so equations to have a minus sign go astray.

Three very basic strategies helped to debug the resulting code. First, I recast the original into a modular version, and added the requisite generalizations in modular fashion. Second, I restricted my updates to a relatively small granularity, keeping a well documented and tested trail of these incremental changes, along with the specific versions of the complete source code for each update. In this fashion, I was always able to back up to any previous status of my code development. And the third strategy, which helped immeasurably in tracking down errors, was the recognition that the solution should be symmetric about the sign of the given source, and the provision for an initial given source of either sign.

5. Demonstration of Reduced-Source Convergence

To illustrate the kind of results obtained by the "xmuh-code" that was extended by the theory of the foregoing sections, two figures, below, show composite plots for 2 runs. Figure 1 displays the behavior of the positive components of the boundary residuals; Figure 2 displays the corresponding behavior of the negative components. Each figure compares the convergence of one run that used 1000 bins for the numerical integrations (and the same number for sampling the reduced sources), and one run that used twice as many bins. In addition, a plot of a traditional inverse-root convergence rate is displayed for illustration. And, to highlight the comparison between the "1000-bin" result and the "2000-bin" result, the "1000-bin" result is additionally shown scaled-down to match the "2000-bin" result at the third iteration. This serves to demonstrate that the convergence rate toward a zero boundary residual is constrained by the precision of the numerical computation.

Whereas the inverse-root improves its convergence by less than a factor of 3 (iterations 3–25), the 1000-bin result improves by 2 orders of magnitude, and the 2000-bin result by more than 3 orders of magnitude. It is important to point out that cpu-time per iteration is constant in a given run, but the magnitude of the constant, of course, depends on the precision of the numerical integration and source-sampling tables (as specified by the refinement of the binning).

A follow-on research note will examine the results, from the reduced-source approach documented herein, in greater detail. In particular, I will examine the rate of convergence to the true solution, using a metric to be developed for that purpose.

Figure 1. Decrease of (positive) reduced-source weight, as a function of iteration number, for a slab of thickness 2 [x-units]. The initial (given) source density was of the form $S(\mu) = \mu e^{-\mu^2}$. Each iteration comprised 50 histories, and, for each of the runs (*i.e.*, using 1000 bins and 2000 bins) individually, the cpu time per iteration was essentially constant. The plots compare how the refinement of the numerical computations affect the rate of decrease, and include a plot of $\frac{constant}{\sqrt{iteration}}$ for illustration.

Figure 2. Decrease of (negative) reduced-source weight, as a function of iteration number, for a slab of thickness 2 [x-units]. The initial (given) source density was of the form $S(\mu) = \mu e^{-\mu^2}$. Each iteration comprised 50 histories, and, for each of the runs (*i.e.*, using 1000 bins and 2000 bins) individually, the cpu time per iteration was essentially constant. The plots compare how the refinement of the numerical computations affect the rate of decrease, and include a plot of $\frac{constant}{\sqrt{iteration}}$ for illustration.

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